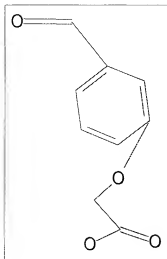


EXHIBIT A



Substance Identification

Beilstein Registry Number	2048742
Beilstein Preferred RN	37748-09-7
CAS Registry Number	37748-09-7
Chemical Name	(3-formyl-phenoxy)-acetic acid
Autoname	(3-formyl-phenoxy)-acetic acid
Molecular Formula	C ₉ H ₈ O ₄
Molecular Weight	180.16
Lawson Number	8629, 1771
Type of Substance	isocyclic
Constitution ID	1856203
Tautomer ID	1952560
Beilstein Reference	0-08-00-00060, 2-08-00-00054, 5-08, 6-08

Field Availability List 1-6

Code	Field Name	Occ.
<u>RX</u>	Reaction	17
<u>CDER</u>	Derivative	4
<u>CPD</u>	Crystal Property Description	1
<u>MP</u>	Melting Point	5
<u>IR</u>	IR Spectroscopy	1
<u>CNR</u>	Reference	16

Reaction 1 of 17

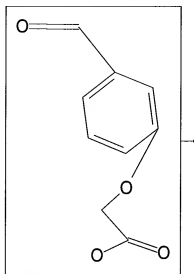
Reaction ID	<u>190141</u>
Reactant BRN	<u>1718733</u> ethanol
Product BRN	<u>2048742</u> (3-formyl-phenoxy)-acetic acid
No. of Reaction Details	<u>2109732</u> (3-formyl-phenoxy)-acetic acid ethyl ester
Reaction Classification	1
Reagent	Preparation
Find similar reactions	HCl
	<u>click here</u>

Note 1
Ref. 1

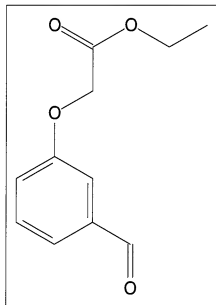
Handbook
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

Reaction 2 of 17

Reaction ID

309586

Reactant BRN

2048742 (3-formyl-phenoxy)-acetic acid

Product BRN

2695071 3-carboxymethoxy-benzoic acid

No. of Reaction Details

1

Reaction Classification

Preparation

Reagent

alkali

water

permanganate

Find similar reactions

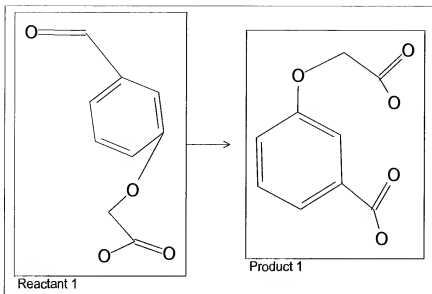
[click here](#)

Note 1

Handbook

Ref. 1

1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reaction 3 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Find similar reactions

558896

2048742 (3-formyl-phenoxy)-acetic acid

385737 acetic acid anhydride

3305754 3-carboxymethoxy-cinnamic acid

1

Preparation

sodium acetate

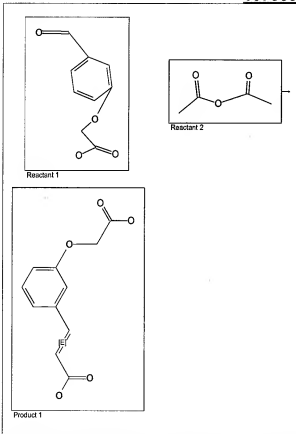
[click here](#)

Note 1

Ref. 1

Handbook

1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reaction 4 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Find similar reactions

636552

2048742 (3-formyl-phenoxy)-acetic acid

505984 acetaldehyde

3279177 [3-(3-oxo-propenyl)-phenoxy]-acetic acid

1

Preparation

diluted NaOH-solution

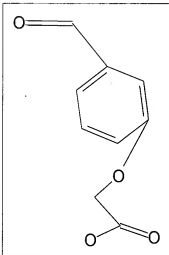
click here

Note 1

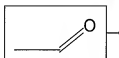
Ref. 1

Handbook

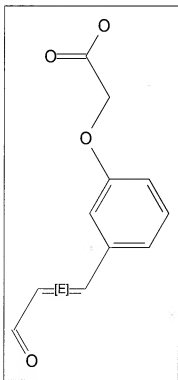
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

Reaction 5 of 17

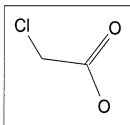
Reaction ID
Reactant BRN

Product BRN
No. of Reaction Details
Reaction Classification
Find similar reactions

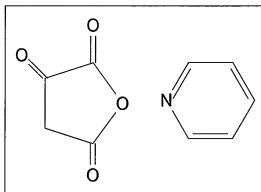
660365
605438 chloroacetic acid
5789338 Pyridinsalz des Oxymaleinsaeureanhydrids
507099 3-hydroxy-benzaldehyde
2048742 (3-formyl-phenoxy)-acetic acid
1
Chemical behaviour
[click here](#)

Note 1
Ref. 1

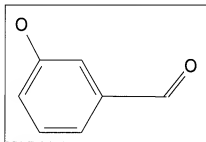
Handbook
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



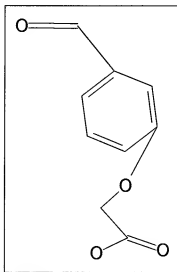
Reactant 1



Reactant 2



Reactant 3



Product 1

Reaction 6 of 17

Reaction ID
Reactant BRN

Product BRN
No. of Reaction Details
Reaction Classification
Reagent

660366
507099 3-hydroxy-benzaldehyde
605438 chloroacetic acid
2048742 (3-formyl-phenoxy)-acetic acid
1
Preparation
NaOH-solution

Find similar reactions

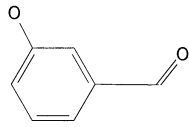
[click here](#)

Note 1

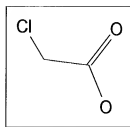
Handbook

Ref. 1

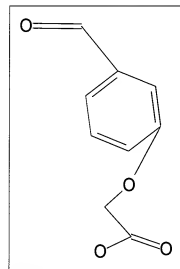
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

Reaction 7 of 17

Reaction ID

2071867

Reactant BRN

5362023 C₁₀H₁₄F₁₂O₂₀

Product BRN

2048742 (3-formyl-phenoxy)-acetic acid

No. of Reaction Details

6173350 C₁₄H₁₇F₁₂O₃₂

Reaction Classification

1

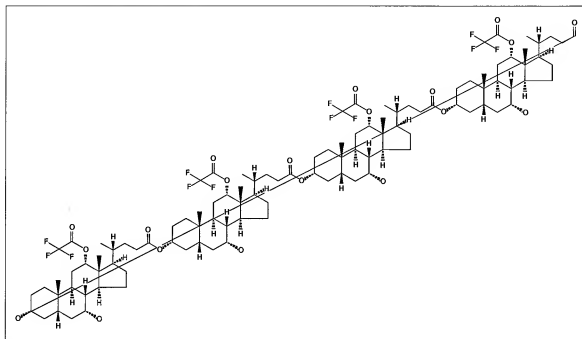
Reagent

Preparation
dicyclohexylcarbodiimide, DMAP
not available

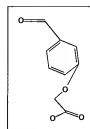
Find similar reactions

Ref. 1

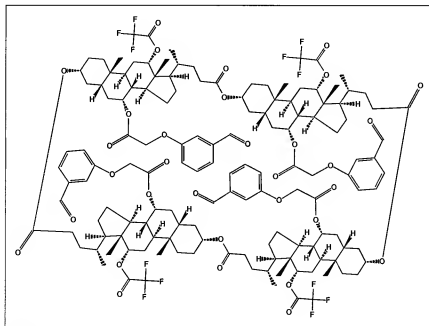
5752565; Journal; Bonar-Law, Richard P.; Mackay, Lindsey G.; Sanders, Jeremy K. M.; JCCCAT; J. Chem. Soc. Chem. Commun.; EN; 5; 1993; 456-458.



Reactant 1



Reactant 2



Product 1

Reaction 8 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Other Conditions

Find similar reactions

4228398

2048742 (3-formyl-phenoxy)-acetic acid

506236 1-nitro-propane

1994538 [3-(2-nitro-but-1-enyl)-phenoxy]-acetic acid

1

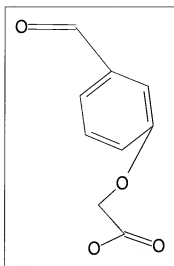
Preparation

(i) nBuNH₂, benzene, (ii) /BRN= 506236/, AcOH

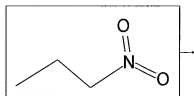
[click here](#)

Note 1

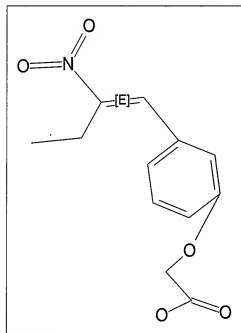
Multistep reaction



Reactant 1



Reactant 2



Product 1

Reaction 9 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Time

Find similar reactions

4510213

2048742 (3-formyl-phenoxy)-acetic acid

1159 pyrrole

7564396 {3-[10,15,20-tris-(3-carboxymethoxy-phenyl)-porphyrinogen-5-yl]-phenoxy}-acetic acid

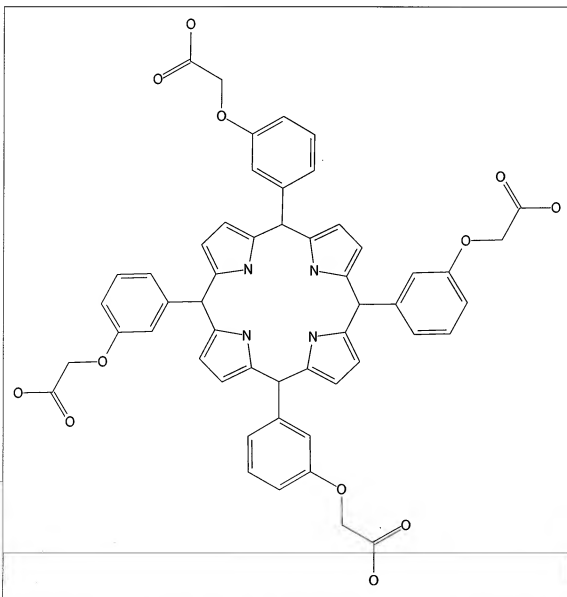
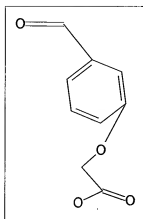
1

Preparation

aq. sodium dodecyl sulfate, HCl

2 hour(s)

click here



Reaction 10 of 17

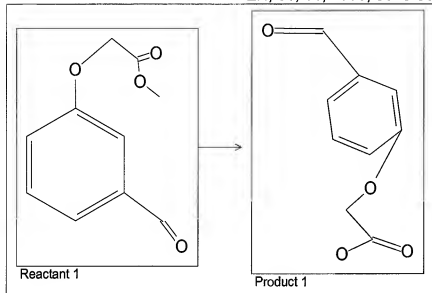
Reaction ID
Reactant BRN
Product BRN
No. of Reaction Details
Reaction Classification
Reagent
Solvent

4517320
1960557 Methyl-m-formyl-phenoxyacetat
2048742 (3-formyl-phenoxy)-acetic acid
1
Preparation
aq. KOH
methanol
tetrahydrofuran
[click here](#)

Find similar reactions

Ref. 1

6021620; Journal; Bonar-Law, Richard P.; JOCEAH; J. Org. Chem.; EN; 61; 11; 1996; 3623-3634.



Reaction 11 of 17

Reaction ID
Reactant BRN
No. of Reaction Details
Reaction Classification
Other Conditions
Find similar reactions

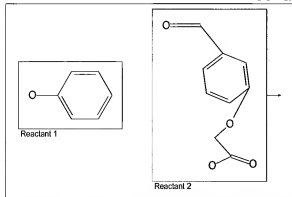
7149987
969616 phenol
2048742 (3-formyl-phenoxy)-acetic acid
1
Chemical behaviour (half reaction)
durch Kondensation
not available

Note 1

Handbook

Ref. 1

1979953; Patent; Hoechst Farb.; DE 362382; FTFVA6; Fortsch. Teerfarbenfabr. Verw. Industriezweige; DE; GE; 14; 1160.

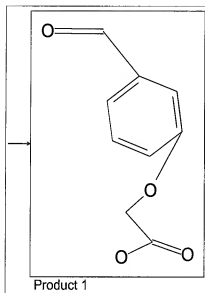


Reaction 12 of 17

Reaction ID
Product BRN
No. of Reaction Details
Reaction Classification
Find similar reactions

7252880
2048742 (3-formyl-phenoxy)-acetic acid
1
Preparation (half reaction)
not available

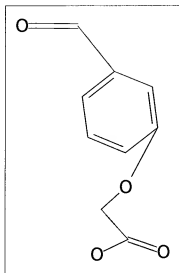
- Ref. 1 **4068762**; Patent; Biorex Lab. Ltd.; DE 2810253; 1978; Chem.Abstr.; EN; 90; 22628.
- Ref. 2 **4084581**; Patent; Ciba-Geigy; DE 2209128; 1972; Chem.Abstr.; EN; 78; 5413.
- Ref. 3 **4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52; 1973; 741,742,743.
- Ref. 4 **2893918**; Patent; Upjohn; US 3944595; 1976; Chem.Abstr.; EN; 85; 176939.
- Ref. 5 **2968330**; Patent; Upjohn; US 3933895; 1974; Chem.Abstr.; EN; 85; 62726.
- Ref. 6 **4384558**; Patent; The Upjohn Co.; US 3933896; 1976; Chem.Abstr.; EN; 85; 32508.
- Ref. 7 **3007991**; Patent; Upjohn Comp.; US 3928417; 1975; Chem.Abstr.; EN; 85; 77744.
- Ref. 8 **4171729**; Patent; The Upjohn Co.; DE 2209990; 1972; Chem.Abstr.; EN; 78; 29477.



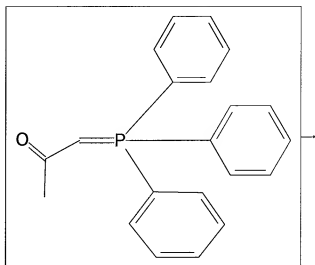
Reaction 13 of 17

Reaction ID
Reactant BRN
Product BRN
No. of Reaction Details
Reaction Classification
Solvent
Other Conditions
Find similar reactions

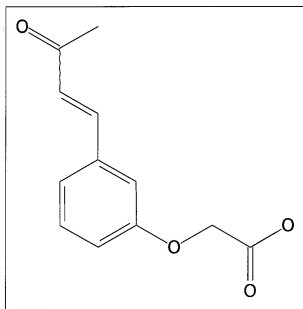
9811771
2048742 (3-formyl-phenoxy)-acetic acid
750077 1-(triphenyl- λ^5 -phosphanylidene)-propan-2-one
9906109 [3-(3-oxo-but-1-enyl)-phenoxy]-acetic acid
1
Preparation
tetrahydrofuran
Heating
[click here](#)



Reactant 1



Reactant 2



Product 1

Reaction 14 of 17

Reaction ID
Reactant BRN

Product BRN
No. of Reaction Details
Reaction Classification
No. of Stages

Stage 1
Stage 2
Reagent

9968144
507099 3-hydroxy-benzaldehyde
506256 bromoacetic acid methyl ester
2048742 (3-formyl-phenoxy)-acetic acid
1
Multistage
2

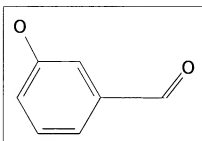
sodium hydroxide

Find similar reactions

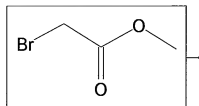
[click here](#)

Ref. 1

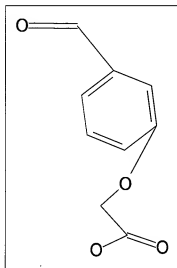
6502017; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael; TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



Reactant 1



Reactant 2



Product 1

Reaction 15 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

No. of Stages

Stage 1

Stage 2

Stage Reactant BRN

Find similar reactions

9969154

2048742 (3-formyl-phenoxy)-acetic acid

1902903 Trimethylsilyldiazomethan

507066 propionic acid anhydride

4652394 hydrocyanic acid; potassium salt

10079086 propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

1

Multistage

2

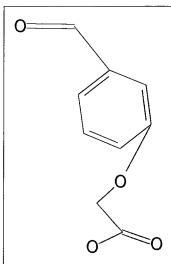
507066 propionic acid anhydride

4652394 hydrocyanic acid; potassium salt

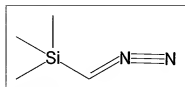
[click here](#)

Ref. 1

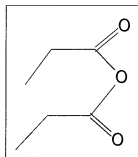
6502017; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael; TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



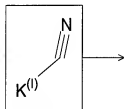
Reactant 1



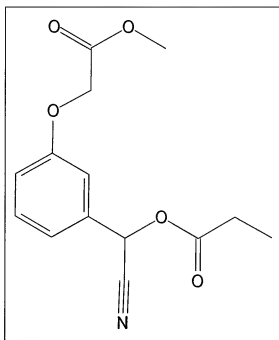
Reactant 2



Reactant 3



Reactant 4



Product 1

Reaction 16 of 17

Reaction ID
Reactant BRN

Product BRN

No. of Reaction Details
Reaction Classification
Find similar reactions

9969155

2048742 (3-formyl-phenoxy)-acetic acid

507066 propionic acid anhydride

1902903 Trimethylsilyldiazomethan

4652394 hydrocyanic acid; potassium salt

10082151 propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

10082152 propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

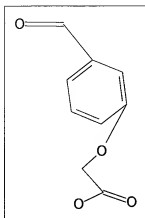
1

Preparation

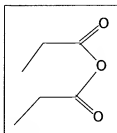
[click here](#)

Note 1
Ref. 1

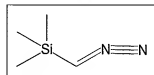
Multistep reaction. Title compound not separated from byproducts
6502017; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael;
TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



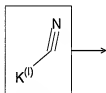
Reactant 1



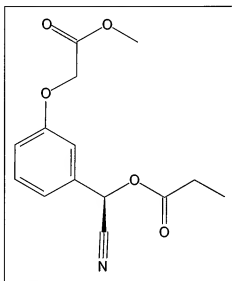
Reactant 2



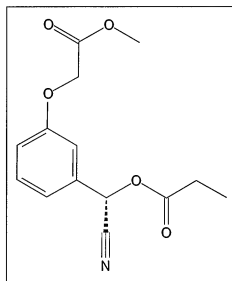
Reactant 3



Reactant 4



Product 1



Product 2

Reaction 17 of 17

Reaction ID
Reactant BRN

Product BRN

No. of Reaction Details
Reaction Classification
Yield
Reagent
Solvent
Other Conditions
Find similar reactions

10200266

195229 1,3,6-trimethyl-5-nitro-1*H*-pyrimidine-2,4-dione

2048742 (3-formyl-phenoxy)-acetic acid

10375693 {3-[2-(1,3-dimethyl-5-nitro-2,6-dioxo-1,2,3,6-tetrahydro-
pyrimidin-4-yl)-vinyl]-phenoxy}-acetic acid

1

Preparation

55 percent (BRN=10375693)

piperidine

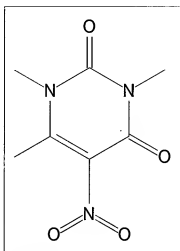
dioxane

Heating

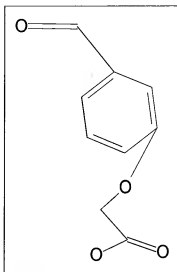
[click here](#)

Ref. 1

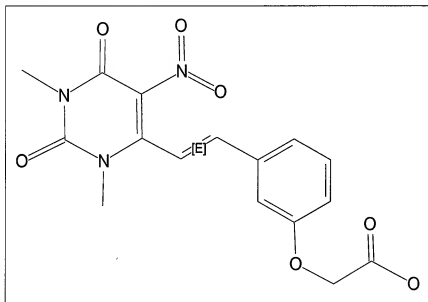
6562381; Journal; Carotti, Angelo; Cadavid, Maria Isabel; Centeno, Nuria B.; Esteve, Cristina; Loza, Maria Isabel; Martinez, Ana; Nieto, Rosa; Ravina, Enrique; Sanz, Ferran; Segarra, Victor; Sotelo, Eddy;



Reactant 1



Reactant 2



Product 1

Derivative 1 of 4

Note 1
Ref. 1

Semicarbazone: F:212-213.5grad (Zers.)
4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;
1973; 741,742,743.

Derivative 2 of 4

Note 1
Ref. 1

Thiosemicarbazone: F:203-204grad
4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;
1973; 741,742,743.

Derivative 3 of 4

Note 1
Ref. 1

2,4-Dinitrophenylhydrazon: F:251.5-252.5grad
4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;
1973; 741,742,743.

Derivative 4 of 4

Note 1
Ref. 1

Ethylester: Kp(2):148-150grad
4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;
1973; 741,742,743.

Crystal Property Description

Colour & Other Properties

Nadeln

Note 1
Ref. 1

Handbook
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.

Melting Point 1-5

VALUE (MP) C	Solvent (.SOL)	Entry Date	Note	Ref.
148 124 - 126 114 - 117 114 - 116 112.5 - 113.5	H2O		1	1 2 3-7 8 9

Note 1
Ref. 1
Ref. 2

Handbook
1970630; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.
4068762; Patent; Biorex Lab. Ltd.; DE 2810253; 1978; Chem.Abstr.;
EN; 90; 22628.

Ref. 3

2893918; Patent; Upjohn; US 3944595; 1976; Chem.Abstr.; EN; 85;
176939.

Ref. 4

2968330; Patent; Upjohn; US 3933895; 1974; Chem.Abstr.; EN; 85;
62726.

Ref. 5

4384558; Patent; The Upjohn Co.; US 3933896; 1976; Chem.Abstr.;
EN; 85; 32508.

Ref. 6

3007991; Patent; Upjohn Comp.; US 3928417; 1975; Chem.Abstr.;
EN; 85; 77744.

Ref. 7

4171729; Patent; The Upjohn Co.; DE 2209990; 1972; Chem.Abstr.;
EN; 78; 29477.

Ref. 8

4084581; Patent; Ciba-Geigy; DE 2209128; 1972; Chem.Abstr.; EN;
78; 5413.

Ref. 9

4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;
1973; 741,742,743.

IR Spectroscopy

Description

Bands

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